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Influence of the elastic field of dilatational nano-disk on the electronic band structure of III-nitride semiconductors

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Introduction

In this study, the influence of non-uniform elastic strain field of the dilatational nano-disk, which is buried in a half-space or in a nanowire (NW), on the electronic band structure of III-nitride semiconductor compounds is investigated. $In_xGa_{1-x}N$ nano-disk has a thickness h corresponding to the lattice constant c in the [0001] direction of the wurtzite crystal structure and the matrix material is assumed to be GaN. The elastic properties of the disk in a half-space or in a NW are studied by using the virtual defect method [1] to account for the boundary conditions at the free surfaces of the matrix material. The **k·p** perturbation theory approach [2], [3] is used to analyze the effect of elastic strains on the conduction band and valence band structure of semiconductors.

Main part

We consider a circular disk $In_xGa_{1-x}N$ with radius r_D = 5 nm and thickness h = 0.56 nm being equal to the lattice constant of the wurtzite crystal structure. The disk is buried in the GaN half-space at a distance d = 30 nm from the free surface or located coaxially to the symmetry axis of the cylindrical NW. The NW has radius r_c=10 nm. The disk is considered to possess a constant dilatational eigenstrain ε^*, which is related to the misfit parameter f caused by the difference in lattice constants of the disk and the surrounding matrix materials.

We explore the virtual defect method [4], [5] to account for the effect of the boundary conditions on the elastic field of the dilatational disk in the elastic medium confined in the half-space or infinite circular cylinder, which models a NW.

We apply the **k·p** perturbation theory approach [2], [3] to study the influence of the strain on the electronic band structure of III-nitride semiconductors. The shift of the edges of the conduction band and valence band due to elastic strains in the vicinity of the nano-disk was studied. The dependences of the shift are plotted in the direction of the symmetry axis Oz of the nano-disk and in the direction perpendicular to this axis. The change in the value of the band gap was also estimated.

Conclusion

The elastic properties of a thin dilatational disk, i.e. nano-disk, in an elastic half-space and an infinitely long NW have been studied. The effect of the strain caused by a nano-disk on the electronic band structure and band gap of the semiconductor has been analyzed. The determining role of the free surface in the change in the electronic band structure of a material caused by an elastic field has been revealed.

References

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